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CONTENTS

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MODELING ENDOHEDRAL FULLERENES IN THE CASE OF THE PHOTOIONIZATION PROCESS

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Abstract
Endohedral fullerenes (EF) $A@C_{60}$ (atom A is confined inside of the carbon fullerene C_{60}) have attracted much attention of investigators in recent years not merely as new, fascinating subjects for studies, but because of an industrial interest in these objects as well. The spectroscopy of the EA is turning into a promising area of new exciting investigations. Because of that, detailed knowledge of the modifications in the structure and photo-spectra of the EA is extremely important.
In this paper are presented some simple models for the theoretical investigations of the photoionization (PI) of the EA and some corresponding results of calculations.

Introduction
The description of the interaction of electromagnetic radiation with an endohedral fullerene is a complicated theoretical problem. Because of that the simplifications of the problem are useful. Here we present two semiempirical models [1,2,3]. They assume that the encaged atom is simulated by a spherical attractive short range potential well V_n (radius R_n, thickness Δ and depth U_n). One of the models [1,2], the Δ - potential model, accounts for the finite thickness Δ of the C_n cage. The other model [3,4,5] is the δ - potential model: C cage is simulate by $\approx \delta(r - R_n)$ ($\Delta = 0$; no interaction between the ground state of the atom and the C cage). The atom A, located well inside $A@C_n$ (denoted by AC) can be easily treated in the Random Phase Approximation (RPA) using the initial step the one-electron Hartree-Fock (HF) method, while the "fullerene-atom A" interaction can be considered as a sort of perturbation [3,4]. In the case of the PI processes the results produced by the both potential models are compared using the frozen cage approximation FCA and dynamical (polarization) cage approximation DCA. In the framework of presented models results in this paper are obtained by the improved version of the RPA method- IPRPA [4].
Atomic units (au) are used throughout the paper.

Models
The following relations gives the differential PI cross section (c.s.) of a spherically-symmetric endohedral shell by non-polarized light [3,5]

$$d\sigma_{n\ell}^{AC}(\omega)/d\Omega = \left[\sigma_{n\ell}^{AC}(\omega)/(4\pi)\right]\left(1 - \beta_{n\ell}^{AC}(\omega)P_2(\cos\theta)/2 + \kappa\gamma_{n\ell}^{AC}(\omega)P_1(\cos\theta) + \right.$$
$$\left. + \kappa\eta_{n\ell}^{AC}(\omega)P_3(\cos\theta)\right)$$

where $\kappa = \omega / c$, P_i are Legendre polynomials, θ is the angle between photon and photoelectron linear momentums, $\beta_{n\ell}$ is the dipole and $\gamma_{n\ell}$, $\eta_{n\ell}$ are non-dipole angular anisotropy parameters (which are defined in [3]) and they are formed by the combination of the dipole D and quadrupole Q matrix elements of photoelectron transitions and photoelectron scattering phases. The cross section $\sigma_{n\ell}^{AC}(\omega)$ is determined by the dipole $D_{nl\to\varepsilon\ell\pm1}^{AC}(\equiv D_{\ell\pm1}^{AC})$ amplitude and is given by the expression [3,4]

$$\sigma_{n\ell}^{AC}(\omega) = (16\pi^2\omega/3c)[(\ell+1)\left|D_{\ell+1}^{AC}\right|^2 + \ell\left|D_{\ell-1}^{AC}\right|^2]$$

where D, Q matrix elements are obtained by solving the RPA (or IPRPA) equations [4] in the framework of the Δ and δ potentials models (defined above).

Results and Conclusisons

In Fig.1. are presented the Xe 5p PI cross sections of $Xe@C_{60}$. This work and other authors calculations [1,4,5] demonstrated that the dynamical screening [1,3,4,5] of the incident radiation by the C_n cage can drastically change the PI cross section compared to the FCA calculations. Present calculations demonstrated that the FCA results of calculated PI c.s. with both potential (δ, Δ) predict a noticeable confinement resonance in the Xe 5p PI c.s. near threshold. The DCA results show the impressive enhancement of the Xe 5p PI cross section compared to the FCA results.

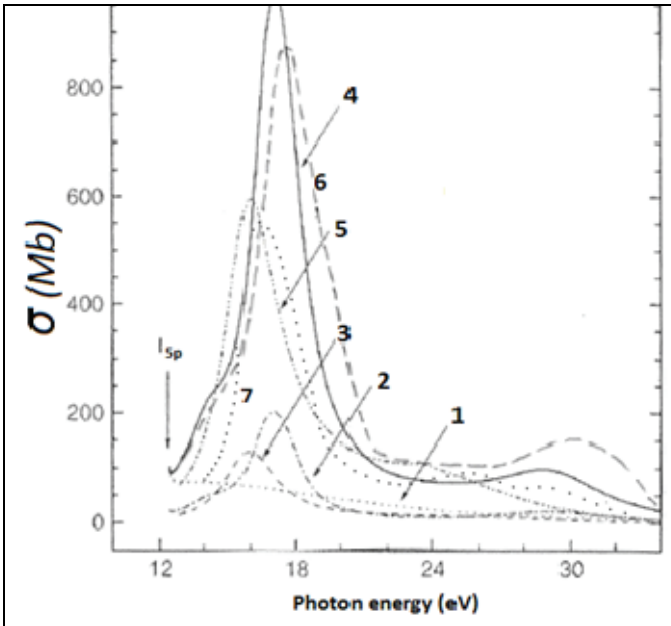

Figure 1. The RPA calculations of the Xe 5p photoionization cross section of AC. 1-PI of free Xe ($\sigma_{5p}^{free}(\omega)$) [1,3,5]; PI in frozen cage approximation of *Xe@C*$_{60}$ [1,5]: 2-$\sigma_{5p}(\omega)-\delta$ model; 3-$\sigma_{5p}(\omega)-\Delta$ model; PI in dynamical cage approximation of *Xe@C*$_{60}$ [1,5]: 4- $\sigma_{5p}(\omega)-\delta$ model; 5-$\sigma_{5p}(\omega)-\Delta$ model; 6,7-this work calculations in IPRPA: $\sigma_{5p}(\omega)-\delta$ model and $\sigma_{5p}(\omega)-\Delta$ model, respectively.

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